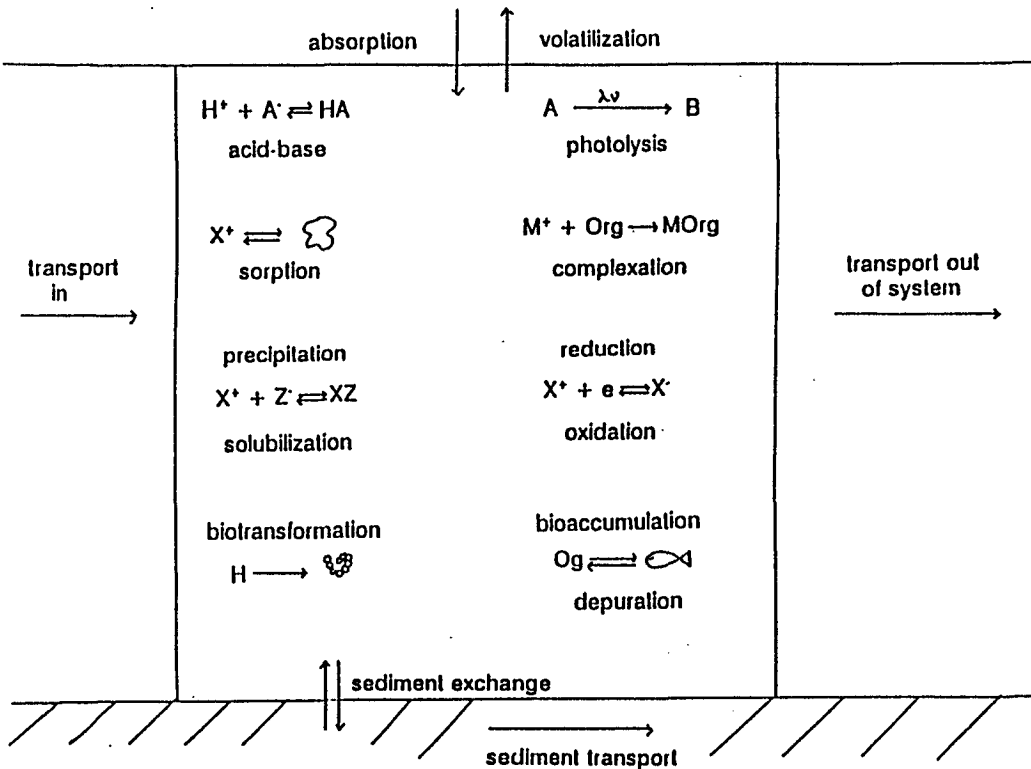




MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: Version 3.0 User's Manual

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Water Quality Modeling ◀ Water Quality vs. Water Chemistry ▶

Most "Water Quality" Models Actually "Water Chemistry" Models
Will Not Predict "Water Quality"

Chemical Composition Not Direct Assessment of Water Quality

Chemical Contaminants Exist in Aquatic Systems in Variety of
Forms, Only Some of Which Are Toxic/Available to Aquatic Life

Generally Cannot Selectively Measure "Toxic" Forms with
Chemical Procedures

Criteria & Standards Developed for Toxic Forms

Total Concentration Grossly Overestimates Toxic Forms

Must Use Bioassays/Toxicity Tests

Factors Affecting Toxicity of Chemical Contaminant to Aquatic Organisms ◀ Water Characteristics ▶

Constituents in Water Can Affect Toxicity of Certain
Chemicals

- Hardness
- Alkalinity
- Suspended Solids & Colloids
- Organics

Tend to Reduce Toxicity of Chemical Contaminants

Toxicity of Chemical Forms

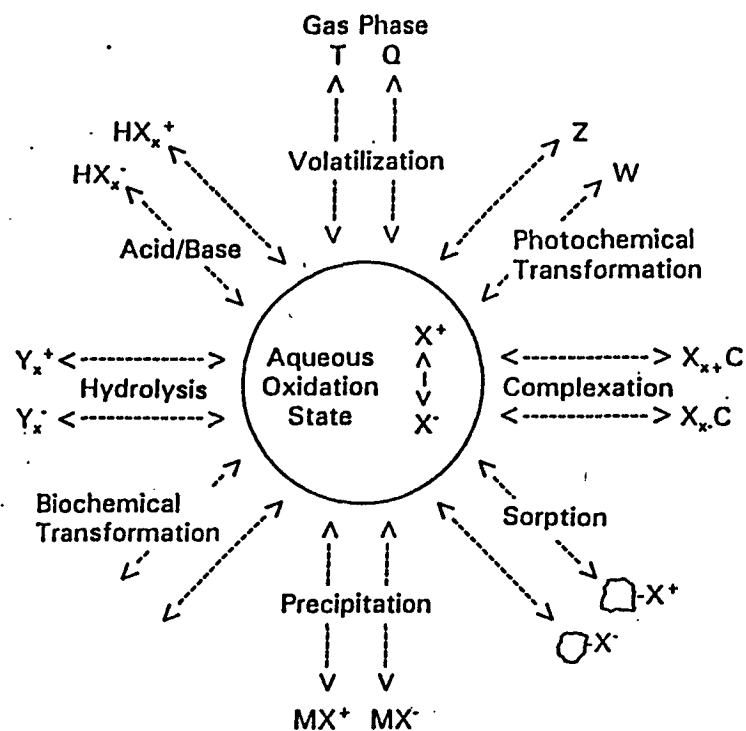
Generally Non-Toxic Forms

- Acids or Their Conjugate Bases
- Precipitates
- Moderate and Strong Complexes
- Sorbed Forms

Generally Toxic Forms

- Aquo Species

Aquatic Chemistry of Chemical Contaminants



Distribution Depends on Kinetics & Thermodynamics of Reactions in a Particular Aquatic System

Each Chemical Species Has Its Own Toxicity Characteristics

Many Forms Are Non-Toxic

Toxic Forms Are Typically Aqueous Aquo-Species of Metals

Examples of Transformation Processes

- Acid-Base -- Proton Transfer



- Precipitation -- Insoluble Compound



- Complexation -- Complex, Chelate, Ion-Dipole Bond



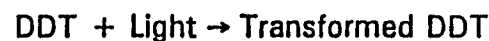
- Redox -- Electron Transfer



- Hydrolysis -- Reaction with Water



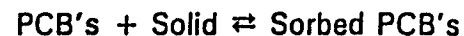
- Phototransformation -- Light



- Vapor Phase Transfer -- Volatilization



- Sorption -- Interaction with Solids (Clays, Dead Organisms, Etc.)



- Biotransformation -- Enzymatic, Biochemical

